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ON OMEGA POLYNOMIAL OF ((4,7)3) NETWORK

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ABSTRACT. The Omega polynomial $\Omega(x)$ was recently proposed by Diudea [*Carpath. J. Math*., 2006, *22*, 43-47]. It is defined on the ground of "opposite edge strips" *ops*. The related polynomial: Sadhana $Sd(x)$ can also be calculated by ops counting. In this paper we compute these polynomials for the ((4,7)3) infinite network, designed by *Trs*(*Ca*(4,4)) sequence of map operations.

Keywords: *polygonal structures, Omega and Sadhana polynomials*

INTRODUCTION

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the covalent bonds. Note that hydrogen atoms are often omitted. Mathematical calculations are necessary in view of exploring important concepts in chemistry. Mathematical chemistry is a branch of theoretical chemistry enabling discussion and prediction of molecular structures or molecular properties, using methods of discrete mathematics, without referring to quantum mechanics. Chemical graph theory is an important tool in the study of molecular structures. This theory had an important impact in the development of chemical sciences.

Let *G*(*V*,*E*) be a connected graph, with the vertex set *V*(*G*) and edge set *E*(*G*). Two edges *e* = *uv* and *f* = *xy* of *G* are called *codistant*, *e co f*, if they obey the following relation [1-3]:

$$d(v,x) = d(v,y)+1 = d(u,x)+1 = d(u,y) \qquad (1)$$

Relation *co* is reflexive, that is, *e co e* holds for any edge *e* of *G*; it is also symmetric, if *e co f* then *f co e*. In general, relation *co* is not transitive, an example showing this fact is the complete bipartite graph $K_{2,n}$. If "*co*" is also transitive, thus an equivalence relation, then *G* is called a *co-graph* and the set of edges $C(e) := \{f \in E(G);\ f\ co\ e\}$ is called an *orthogonal cut oc* of *G*, *E*(*G*) being the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup ... \cup C_k,\ C_i \cap C_j = \varnothing, i \neq j$. Klavžar [4] has shown that relation *co* is a theta Djoković-Winkler relation [5,6].

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Let $e = uv$ and $f = xy$ be two edges of G which are *opposite* or topologically parallel and denote this relation by *e op f*. A set of opposite edges, within the same face/ring, eventually forming a strip of adjacent faces/rings, is called an *opposite* edge *strip*, *ops*, which is a quasi-ortogonal cut *qoc* (*i. e*., the transitivity relation is not necessarily obeyed). Note that *co* relation is defined in the whole graph while *op* is defined only in a face/ring. The length of *ops* is maximal irrespective of the starting edge.

Let $m(G, s)$ be the number of *ops* strips of length s. The Omega polynomial is defined as [1]

$$\Omega(x) = \sum_{s} m(G,s) \cdot x^{s} \tag{2}$$

The first derivative (in x=1) equals the number of edges in the graph

$$\Omega'(1) = \sum_{s} m(G,s) \cdot s = e = |E(G)| \tag{3}$$

A topological index, called Cluj-Ilmenau [2], CI=$CI(G)$, was defined on Omega polynomial

$$CI(G) = \{[\Omega'(1)]^2 - [\Omega'(1) + \Omega''(1)]\} \tag{4}$$

The Sadhana index $Sd(G)$ was defined by Khadikar *et al*. [7,8] as

$$Sd(G) = \sum_{s} m(G,s)(|E(G)| - s) \tag{5}$$

where $m(G,s)$ is the number of strips of length s. The Sadhana polynomial $Sd(G,x)$ was defined by Ashrafi *et al*. [9]

$$Sd(G,x) = \sum_{s} m(G,s) \cdot x^{|E(G)|-s} \tag{6}$$

Clearly, the Sadhana polynomial can be derived from the definition of Omega polynomial by replacing the exponent s by $|E(G)\text{-}s|$. Then the Sadhana index will be the first derivative of $Sd(x)$ evaluated at x = 1.

The aim of this study is to compute the Omega and Sadhana polynomials of the ((4,7)3) infinite network. This network can be seen as a modification of the graphene sheet [10-12].

RESULTS AND DISCUSSION

The design of ((4,7)3) network can be achieved by *Trs*(*Ca*(4,4)) sequence of map operations [13-16], where *Ca* is the pro-chiral “Capra” operation and *Trs* is the truncation operation, performed on selected atoms (those having the valence four); (4,4) is the Schläfli symbol [17] for the planar net made by squares and vertices of degree/valence four, which was taken as a ground for the map operations. Figure 1 illustrates the ((4,7)3) pattern. Since any net has its co-net, depending of the start/end view, the co-net of ((4,7)3) net (Figure 2) will also be considered.

Looking to these nets, one can see that there are $k^2+(k-1)^2$ squares in the net and $4k(k-1)$ in co-net, k being the number of repeat units. This implies there exactly exist $2(k^2+(k-1)^2)$ strips of length 2 in the net and $8k(k-1)$ in co-net and the others are of length 1. By definition of Omega polynomial, the formulas for the two polynomials and derived indices (Table 1) can be easily obtained. Some examples to prove the above formulas are collected in Table 2.

Figure 1. The 2-dimensional ((4,7)3) net (3×3 units) designed by the sequence of map operations *Trs*(*Ca*(4,4)): non-optimized (left) and optimized (right) structure.

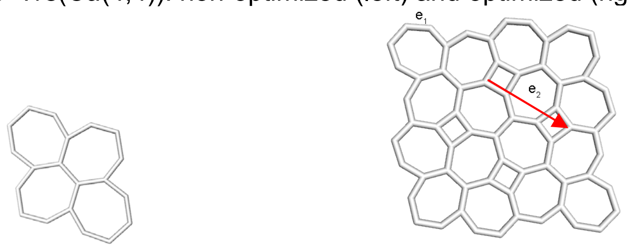

Figure 2. The ops strips of length s=1 and s=2 in the 2-dimensional co-net (the repeat unit (left) and 2×2 units (right) of ((4,7)3) pattern

Table 1. Omega and Sadhana polynomials in the ((4,7)3) modified graphene

Structure	Formulas
Net	$\Omega(x) = 2[k^2 + (k-1)^2]\cdot x^2 + (10k^2 + 14k - 4)\cdot x$
	$\Omega'(1) = 18x^2 + 6k = 6k(3k+1) = e(G)$
	$CI(G) = 2(162k^4 + 108k^3 + 5k^2 + k - 2)$
	$Sd(x) = 2[k^2 + (k-1)^2]\cdot x^{18k^2+6k-2} + (10k^2 + 14k - 4)\cdot x^{18k^2+6k-1}$
	$Sd'(1) = 6k(3k+1)(14k^2 + 10k - 3) = e\cdot(14k^2 + 10k - 3)$
	$Sd(G) = Sd'(1) = 252x^4 + 264x^3 + 6k^2 - 18k$
	$v(G) = 4k(5 + 3(k-1))$
Co-Net	$\Omega(x) = 4k(k-1)\cdot x^2 + (10k^2 + 14k - 1)\cdot x$
	$\Omega'(1) = 18x^2 + 6k - 1 = e(G)$
	$CI(G) = 2(162k^4 + 108k^3 - 13k^2 - 5k + 1)$
	$Sd(x) = 4k(k-1)\cdot x^{18k^2+6k-3} + (10k^2 + 14k - 1)\cdot x^{18k^2+6k-2}$
	$Sd'(1) = 2(7k^2 + 5k - 1)(18k^2 + 6k - 1) = 2(7k^2 + 5k - 1)\cdot e$
	$Sd(G) = Sd'(1) = 252x^4 + 264x^3 + 10k^2 - 22k + 2$
	$v(G) = 4k(5 + 3(k-1))$

Table 2. Examples for the formulas in Table 1.

k	Omega polynomial	*v*(*G*)	*e*(*G*)	*CI*(*G*)	*Sd*(*G*)
	Net				
2	$64X+10X^2$	64	84	6952	6132
3	$128X+26X^2$	132	180	32168	27540

k	Omega polynomial	*v*(*G*)	*e*(*G*)	*CI*(*G*)	*Sd*(*G*)
4	$212X+50X^2$	224	312	96932	81432
5	$316X+82X^2$	340	480	229756	190560
6	$440X+122X^2$	480	684	466928	383724
7	$584X+170X^2$	644	924	852512	695772
	Co-Net				
2	$67X+8X^2$	64	83	6790	6142
3	$131X+24X^2$	132	179	31814	27566
4	$215X+48X^2$	224	311	96314	81482
5	$319X+80X^2$	340	479	228802	190642
6	$443X+120X^2$	480	683	465566	383846
7	$587X+168X^2$	644	923	850670	695942

CONCLUSIONS

Omega and Sadhana polynomials are useful theoretical tools in describing polygonal structures, such as the modified graphene of ((4,7)3) pattern. This modification can be acheved by using sequences of map operations.

Formulas to calculate the above polynomials and derived indices in an infinite ((4,7)3) lattice were given, along with some examples.

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